

Product Name: Embelin

Catalog No.: 2156

Batch No.: 1

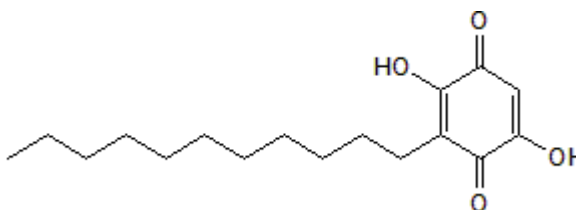
CAS Number: 550-24-3

EC Number: 208-979-8

IUPAC Name: 2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₆O₄
Batch Molecular Weight: 294.39
Physical Appearance: Dark orange solid
Solubility: ethanol to 10 mM with gentle warming
 DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >98% purity
¹H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.36	8.9	
Found	69.4	9.04	

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione

Description:

Cell-permeable, non-peptide inhibitor of X-linked inhibitor of apoptosis (XIAP) (IC_{50} = 4.1 μ M in competition binding assay with Smac peptide); binds to the BIR3 domain, preventing XIAP interaction with caspase-9 and Smac. Inhibits cell growth, induces apoptosis and activates caspase-9 in prostate cancer cells (IC_{50} 4 - 6 μ M), but has a weaker effect on normal prostate cells (IC_{50} = 19 - 20 μ M). Overcomes the protective effect of XIAP on apoptosis in XIAP-transfected Jurkat cells. Anti-tumor, analgesic and anti-inflammatory in vivo.

Physical and Chemical Properties:

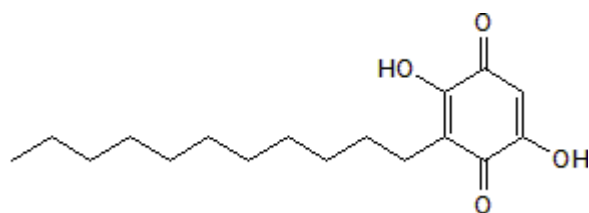
Batch Molecular Formula: $C_{17}H_{26}O_4$

Batch Molecular Weight: 294.39

Physical Appearance: Dark orange solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

ethanol to 10 mM with gentle warming
DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Chitra et al (1994) Antitumor, anti-inflammatory and analgesic property of embelin, a plant product. *Chemotherapy* **40** 109. PMID: 7510605.

Nikolovska-Coleska et al (2004) Discovery of embelin as a cell-permeable, small-molecular weight inhibitor of XIAP through structure-based computational screening of a traditional herbal medicine three-dimensional structure database. *J.Med.Chem.* **47** 2430. PMID: 15115387.

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